Dynamical error bounds for continuum discretisation via Gauss quadrature rules, – a Lieb-Robinson bound approach

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Instances of discrete quantum systems coupled to a continuum of oscillators are ubiquitous in physics. Often the continua are approximated by a discreate set of modes. We derive error bounds on expectation values of system observables that have been time evolved under such discretised Hamiltonians. These bounds take on the form of a function of time and the number of discrete modes, where the discrete modes are chosen according to Gauss quadrature rules. The derivation makes use of tools from the field of Lieb-Robinson bounds and the theory of orthonormal polynominals.

Instances of discrete quantum systems coupled to continua are ubiquitous in physics as they describe open quantum systems, i.e. well-characterised systems under the control of the experimenter that are in contact with a much larger and typically uncontrolled environment[1]. Examples can be found in quantum optics[2], solid state and condensed matter physics[3] and recently quantum biology[4,5] to name just a few. In numerical studies environments with continuous spectra are often modeled by a discrete spectrum while in analytical work the reverse, i.e. replacing a discrete environmental spectrum by a continuous one in a "continuum limit"[3], is often convenient. There have been many suggestions about how to best approximate continuous spectra by discrete spectra for the evaluation of dynamical quantities and numerical studies into their efficiency. These studies were, to the best of our knowledge, initiated by Rice in 1929[6–8] in which the continuum was discretised to form a point spectrum with support at equally spaced points. Later, it was suggested by Burkey and Cantrell[9] that a different choice of discretisation would lead to a more accurate description of the dynamics. This later idea was based on the fact that approximating integrals by discrete sums using Gauss quadrature rules is often more efficient than the trapezoidal rule. A bibliographical review of the subject can be found in[10]. While sometimes estimates to some of the committed errors are given[9,11], exact bounds for the quantity

$$\left|\mathrm{tr}\left[\hat{O}\mathrm{e}^{-\mathrm{i}t\hat{H}_{\mathrm{con}}}\hat{\varrho}_0\mathrm{e}^{\mathrm{i}t\hat{H}_{\mathrm{con}}}\right]-\mathrm{tr}\left[\hat{O}\mathrm{e}^{-\mathrm{i}t\hat{H}_{\mathrm{dis}}}\hat{\varrho}_0\mathrm{e}^{\mathrm{i}t\hat{H}_{\mathrm{dis}}}\right]\right|, \tag{1}$$

where $\hat{O}$ is an observable, $\hat{\varrho}_0$ is any initial state of potential interest, $\hat{H}_{\mathrm{con}}$ is a Hamiltonian with absolutely continuous spectra and $\hat{H}_{\mathrm{dis}}$ is a Hamiltonian with pure point spectra, do not appear to exist in the literature. Bounds of this form are of particular relevance because they concern precisely the quantities of physical interest – the expectation values of local observables. In this article, we will derive bounds on the quantity Eq. (1) for physically relevant unbounded Hamiltonians, for discretisation schemes based on Gauss quadrature rules.

In a different vein of research, in the context of lattice quantum systems, a bound introduced by Lieb and Robinson[12] provides a measure for the speed of propagation of signals in a spatially extended spin quantum system with finite range interaction, and bounds the decay of the magnitude of signals propagating faster than this speed. The bound has been an indispensable tool to prove many intriguing properties of many-body Hamiltonians and their ground and thermal states, such as, e.g., the Lieb-Schulz-Mattis theorem[13,14], exponential clustering of correlations[15,16], area laws for entanglement[17,18], efficient approximations of ground and thermal states and dynamics[19–21], and speed limits on the distribution of correlations and entanglement[22–24]. Naturally, since the

original statement of the bound in 1972, there have been many refinements and generalizations, see, e.g.,[25–30] and references therein.

More precisely, the Lieb-Robinson bound states that there is a velocity $v > 0$ and constants $\mu > 0$ and $K > 0$, which depend on the details of the lattice and the Hamiltonian, such that the operator norm $\|\cdot\|$ of the commutator of two local observables $\hat{A}$ and $\hat{B}$, separated by a distance $|x|$, is bounded by

$$\|[e^{\mathrm{i}\hat{H}t}\hat{A}e^{-\mathrm{i}\hat{H}t}, \hat{B}]\| \leq K\|\hat{A}\|\|\hat{B}\|e^{-\mu(|x|-vt)}. \tag{2}$$

Often, the development of a new Lieb-Robinson bound goes hand in hand with the development of new physical theorems. Here we show that the newly developed Lieb-Robinson bound in[31], has an application in an area of research which has, up to now, only been probed numerically. Namely, it will be one of two key ingredients in our proof of bounds for Eq. (1). The other key ingredient, will be a unitary transformations based on the theory of orthogonal polynomials from a non-local Hamiltonian to a local one (an infinite lattice with local coupling), to which a Lieb-Robinson bound applies. These two ingredients will be combined to achieve the desired result. First, the non-local Hamiltonian will be written as an infinite lattice with local interaction via a unitary operation. Secondly, this lattice will be spatially truncated and the Lieb-Robinson bound will be applied to estimate the error involved in the truncation. Finally, a unitary transformation will be applied to the truncated lattice to write it in the form of the desired discretised (non-local) Hamiltonian. When viewed from the perspective of the discretised non-local Hamiltonian, the Lieb-Robinson distance $|x|$ (described in Eq. (2)) will no longer play the role of a distance, but instead; will determine the number of pure point spectra sampled from the continuum.

I. THE HAMILTONIAN

In this section we define the Hamiltonians we will be considering in this article[32]. We consider a quantum system coupled to a bosonic bath. The Hilbert space $\mathcal{S}$ of the system carries a "free" Hamiltonian $\hat{H}_{\mathcal{S}}$, while the bosonic bath is described by the Fock space $\mathcal{B} := \Gamma(\mathfrak{h})$ over the mode Hilbert space $\mathfrak{h}$, with the free Hamiltonian $d\hat{\Gamma}(G)$ arising from the second quantization of the positive self-adjoint operator G on $\mathfrak{h}$. The coupling is via one mode $h \in \mathfrak{h}$ and a bounded in operator norm self-adjoint system operator $\hat{A}_{\mathcal{S}}$, so that altogether we have on $\mathcal{S} \otimes \mathcal{B}$ the Hamiltonian

$$\hat{H} = \hat{H}_{\mathcal{S}} \otimes \mathbb{1}_{\mathcal{B}} + \mathbb{1}_{\mathcal{S}} \otimes d\hat{\Gamma}(G) + \hat{A}_{\mathcal{S}} \otimes \hat{\Phi}(h), \tag{3}$$

where $\hat{\Phi}$ denotes the usual field operator. G is a function g of momentum variables k (known as the *dispersion relation*), and can be expressed in terms of bath creation and annihilation operators as

$$d\hat{\Gamma}(G) = \int dk\ g(k) a_k^\dagger a_k \tag{4}$$

and

$$\hat{\Phi}(h) = \int dk\ h(k)\big(a_k^\dagger + a_k\big). \tag{5}$$

The form Eq. (3) is often referred to as a Pauli-Fierz Hamiltonian[33], specialized in our case by allowing one interaction term. We note that although $\hat{A}_{\mathcal{S}}$ is bounded, there are no constraints on the system Hamiltonian $\hat{H}_{\mathcal{S}}$, it can be unbounded or otherwise and comprise of bosons, fermions, spins etc. Definining the *free* Hamiltonian as $\hat{H}_0 = \hat{H}_{\mathcal{S}} \otimes \mathbb{1}_{\mathcal{B}} + \mathbb{1}_{\mathcal{S}} \otimes d\hat{\Gamma}(G)$, Eq. (3) is well defined on $\mathcal{D}(\hat{H}) = \mathcal{D}(\hat{H}_0)$ if[34]

$$\int \frac{h^2(k)}{g(k)} dk < \infty. \tag{6}$$

It includes the spin-boson-Model achieved by letting $\mathcal{S} = \mathbb{C}^2$, $\hat{H}_{\mathcal{S}} = \alpha\hat{\sigma}_z$, and $\hat{A}_{\mathcal{S}} = \hat{\sigma}_x$, where α is a positive constant and $\hat{\sigma}_x, \hat{\sigma}_z$ are the Pauli matrices. Let $E(dx)$ be the projection valued spectral measure of G. Then we form the scalar measure

$$\mu_0(d\omega) = \langle h, E(d\omega)h \rangle\ . \tag{7}$$

The measure is absolutely continuous with respect to the Lebesgue measure, and we can write $\mu_0(dx) = \pi^{-1} J(x) dx$ with the *spectral density*[35] J. When g is monotone, it is defined as

$$J(\omega) = \pi h\left(g^{-1}(\omega)\right)^2 \left|\frac{dg^{-1}(\omega)}{d\omega}\right|, \tag{8}$$

where g^{-1} is the inverse of g. If g is not monotone, we would additionally have a sum over inverse images $g^{-1}(\{\omega\})$, and when the momentum variable has more dimensions, we would also have an integral over the inverse image. The minimally closed interval containing its support is $[\omega_{min}, \omega_{max}]$ with $\omega_{min} := \inf\ g \geq 0$, $\omega_{max} := \sup\ g$. The case $\omega_{min} = 0$ is called *massless* where as $\omega_{min} > 0$ is known as *massive*. We will be dealing with the case $\omega_{max} < \infty$, hence $\mu_0(dx)$ is determinate with all moments finite (see e.g.[36]). For later purposes, it will be convenient to recall that Hamiltonian Eq. (3) is isomorphic to the so-called *standard form* defined on page 5 of[37]. We summarise this standard form here, for the convenience of the reader. We observe that the bath in Hamiltonian Eq. (3) is fully specified by the triple $(\mathfrak{h}, G, h)$. Suppose now we have another environment system $(\tilde{\mathfrak{h}}, \tilde{G}, \tilde{h})$ and a unitary operator $U : \mathfrak{h} \to \tilde{\mathfrak{h}}$ such that $Uh = \tilde{h}$ and

$UGU^\dagger = \tilde{G}$. Under such an isomorphism all the details of system-environment are mapped into each other. This is formally done by the unitary operator $\hat{\Gamma}(U) : \Gamma(\tilde{\mathfrak{h}}) \to \Gamma(\tilde{\mathfrak{h}})$. Note that the scalar measure Eq. (7) is invariant under this isomorphisum U. In fact, it completely determines the triple $(\mathfrak{h}, G, h)$ up to an isomorphisum. Indeed, we are permitted to set

$$\begin{aligned} \tilde{\mathfrak{h}} &= L^2(\mathbb{R}^+, \mu), \\ (\tilde{G}\psi)(x) &= x\psi(x) \ \ \forall\, \psi \in \tilde{\mathfrak{h}}, \\ \tilde{h}(x) &= 1. \end{aligned} \tag{9}$$

The unitary operator defining the isomorphism is given by $\left(U\mathrm{e}^{\mathrm{i}tG}h\right)(x) = \mathrm{e}^{\mathrm{i}tx}$. The triple $(\tilde{\mathfrak{h}}, \tilde{G}, \tilde{h})$ defined by Eq. (9), is referred to as the Standard form of $(\mathfrak{h}, G, h)$. We observe that when Eqs. (4) and (5) are written in standard form, k is a scalar. We will use the standard form in theorems 1 and 2.

II. DISCRETISATION OF THE CONTINUOUS BATH

Let $P_n(x)$ be the real orthonormal polynomial of order n with respect to the measure $\mu_0(dx) = \pi^{-1}J(x)dx$ so that

$$\int \mu_0(dx) P_n(x) P_m(x) = \delta_{m,n}, \quad n, m \in \mathbb{N}_0. \tag{10}$$

The existence and uniqueness (up to a real phase) of these orthonormal polynomials is well established[38]. We can use them to define a discretised Hamiltonian

$$\hat{H}_L = \hat{H}_{\mathcal{S}} \otimes \mathbb{1}_{\mathcal{B}} + \hat{A}_{\mathcal{S}} \otimes \sum_{n=1}^{L} h_n^{(L)}(c_n^\dagger + c_n) + \mathbb{1}_{\mathcal{S}} \otimes \sum_{n=1}^{L} \omega_n^{(L)} c_n^\dagger c_n, \quad L \in \mathbb{N}_+ \tag{11}$$

where $\omega_n^{(L)}$ are the zeros of $P_L(x)$ and

$$h_n^{(L)} = \frac{1}{\sqrt{\sum_{k=0}^{L-1} P_k^2(\omega_n^{(L)})}}. \tag{12}$$

The c_n ($c_m^\dagger$) on $\mathcal{B}$ are bosonic annihilation (creation) operators (and can be expressed in terms of the field operators of Hamiltonian Eq. (3) as detailed by Eq. (68) in the proof). The discretised Hamiltonian, Eq. (11) has a nice interpretation in terms of Gauss quadrature rules: $\{\omega_n^{(L)}\}_{n=1}^L$ are the Gauss knots and $\{(h_n^{(L)})^2\}_{n=1}^L$ are the Gauss weights for the weight function $J(\cdot)/\pi$ (see section 1.4.2 for an introduction to Gauss quadrature and last paragraph of section 1.4.1 and Eq.

(3.1.7) for the nodes and weights[38]). What is more, the theory of orthogonal polynomials has established that $\omega_{min} \leq \omega_n^{(L)} \leq \omega_{max}$ for all L, n and $\{\omega_n^{(L)}\}_{n=1}^{L}$ interlace $\{\omega_n^{(L+1)}\}_{n=1}^{L+1}$:

$$\omega_{L+1}^{(L+1)} < \omega_L^{(L)} < \omega_L^{(L+1)} < \omega_{L-1}^{(L)} < \ldots < \omega_1^{(L)} < \omega_1^{(L+1)}, \tag{13}$$

thus discretisation in terms of the zeros of orthogonal polynomials corresponds to a natural way of discretising a continuum. We note that the spectral density of Hamiltonian Eq. (11) forms a pure point measure. This is in stark contrast with the spectral density of Hamiltonian Eq. (3), which is the weight function of an absolutely continuous measure with respect to the Lebesgue measure.

This discretisation will lead to errors in time evolved observables on the system degrees of freedom that can be bounded as determined by the following theorem. For self-adjoint operators of the form $\hat{O} = \hat{O}_{\mathcal{S}} \otimes \mathbb{1}_{\mathcal{B}}$, $\hat{O}_{\mathcal{S}} \in \mathcal{S}$ and initial normalised quantum states $\hat{\varrho}_0$ on $\mathcal{S} \otimes \mathcal{B}$ we find the following result.

Theorem 1. *For any system observable $\hat{O}$, $\|\hat{O}\| < \infty$ the error introduced on its expectation value at any time $t \geq 0$ when it's dynamics are approximated by the discretised Hamiltonian $\hat{H}_L$, is bounded by*

$$\begin{aligned} &\left|\mathrm{tr}\left[\hat{O}\mathrm{e}^{-\mathrm{i}t\hat{H}}\,\hat{\varrho}_0\mathrm{e}^{\mathrm{i}t\hat{H}}\right] - \mathrm{tr}\left[\hat{O}\mathrm{e}^{-\mathrm{i}t\hat{H}_L}\,\hat{\varrho}_0\mathrm{e}^{\mathrm{i}t\hat{H}_L}\right]\right|^2 \\ &\leq 8\eta_0\|\hat{O}\|^2\frac{\|\hat{A}_{\mathcal{S}}\|}{\omega_{max}}\frac{(\omega_{max}t)^{L+1}}{(L+1)!}\left(\mathrm{e}^{\omega_{max}t}+1\right)\left(\|\vec{\gamma}_0\|^{1/2}+\eta_0\|\hat{A}_{\mathcal{S}}\|t\right), \end{aligned} \tag{14}$$

for $L = 1, 2, 3, \ldots$ where $\eta_0 = \sqrt{\frac{2}{\pi}\int dx J(x)}$, and the operator $\vec{\gamma}_0$ encodes information regarding 2-point correlation functions in $\mathcal{B}$ of the initial state. More precisely,

$$\vec{\gamma}_0 = \begin{pmatrix} \vec{\gamma}_{xx} & \vec{\gamma}_{xp} \\ \vec{\gamma}_{px} & \vec{\gamma}_{pp} \end{pmatrix}, \tag{15}$$

where $[\vec{\gamma}_{xx}]_{n,m} = \mathrm{tr}[\hat{x}_n\hat{x}_m\hat{\varrho}_0]$, $[\vec{\gamma}_{xp}]_{n,m} = \mathrm{tr}[\hat{x}_n\hat{p}_m\hat{\varrho}_0]$, $[\vec{\gamma}_{px}]_{n,m} = \mathrm{tr}[\hat{p}_n\hat{x}_m\hat{\varrho}_0]$, $[\vec{\gamma}_{pp}]_{n,m} = \mathrm{tr}[\hat{p}_n\hat{p}_m\hat{\varrho}_0]$, $n, m \in \mathbb{N}_+$ *with*

$$\begin{aligned} \hat{x}_n &= \frac{1}{\sqrt{2}}\int \mu_0^{(1/2)}(dx)P_{n-1}(x)\left(a_x^\dagger + a_x\right), \\ \hat{p}_n &= \frac{\mathrm{i}}{\sqrt{2}}\int \mu_0^{(1/2)}(dx)P_{n-1}(x)\left(a_x^\dagger - a_x\right), \quad n \in \mathbb{N}_+ \end{aligned} \tag{16}$$

on $\mathcal{B}$ where $\mu_0^{(1/2)}(dx) := \sqrt{J(x)/\pi}\,dx$. Here $\hat{x}_n$ and $\hat{p}_n$ have been written in standard form (see section I).

See section VI A for the proof of this theorem and appendix A 1 for alternative expressions for $\|\vec{\gamma}_0\|$ and examples including when $\mathrm{tr}_{\mathcal{S}}[\hat{\varrho}_0]$ is the vacuum state.

Theorem 1 provides, to the best of our knowledge, for the first time, a bound on the error that results from approximating a bath with absolutely continuous spectrum by a bath with pure point spectrum in the form of a sum over discrete modes and vice versa. The Lieb-Robinson light cone is achieved by choosing a tangent surface to the r.h.s. of Eq. (14) bounding this non-linear function from above. Prior to this work discretisations of continuum baths had a long history of being probed numerically (see[9,11,39–41] and references here in). A fundamental insight was provided by Burkey and Cantrell when they numerically observed that using the evenly spaced knots specified by the trapezoid rule (which is referred to as *Rice discretization*) seems not to be the most efficient way to discretise a continuum[9]. As pointed out in[40], their choice of Gauss quadrature rules to discretise the continuum is for the weight function $J(\cdot)/\pi$, and thus theorem 1 applies to it. We will thus refer to the particular choice of Gauss weights and knots in Eq. (11) as *Burkey-Cantrell* discretisation.

However, Eq. (11) is not the unique way to use Gauss quadrature rules to discretise the continuum. The next theorem will present a sharper bound compared to that of Eq. (14) by discretising the bath according to the weight function $J(\sqrt{\cdot})/\pi$ instead. Via a trivial change of variable followed by using the properties of $\mu_0(dx)$, one verifies that the measure

$$\mu_1(dx) := \pi^{-1} J(\sqrt{x}) dx, \tag{17}$$

is determinate, with all moments finite. Again, we define $P'_n(x)$ as the real orthonormal polynomial of order n with respect to the measure $\mu_1(dx)$:

$$\int \mu_1(dx) P'_n(x) P'_m(x) = \delta_{m,n}, \quad n, m \in \mathbb{N}_0. \tag{18}$$

We use these orthogonal polynomials to define a discretised Hamiltonian:

$$\hat{H}'_L = \hat{H}_{\mathcal{S}} \otimes \mathbb{1}_{\mathcal{B}} + \hat{A}_{\mathcal{S}} \otimes \sum_{n=1}^{L} \frac{h_n'^{(L)}}{\sqrt{2\bar{\omega}_n^{(L)}}} (c_n'^{\dagger} + c'_n) + \mathbb{1}_{\mathcal{S}} \otimes \sum_{n=1}^{L} \bar{\omega}_n^{(L)} c_n'^{\dagger} c'_n, \quad L \in \mathbb{N}_+ \tag{19}$$

where $\bar{\omega}_n^{(L)} = \sqrt{\omega_n'^{(L)}}$, $\omega_n'^{(L)}$ are the zeros of $P'_L(x)$ and

$$h_n'^{(L)} = \frac{1}{\sqrt{\sum_{k=0}^{L-1} P_k'^2(\omega_n'^{(L)})}}. \tag{20}$$

c'_i ($c'^{\dagger}_j$) on $\mathcal{B}$ are bosonic annihilation (creation) operators (and can be expressed in terms of the field operators of Hamiltonian Eq. (3) as detailed by Eq. (69) in the proof that is found in section 8.).

Here $\{\omega_n'^{(L)}\}_{n=1}^L$ are the Gauss knots and $\{(h_n'^{(L)})^2\}_{n=1}^L$ are the Gauss weights for the weight function $J(\sqrt{\cdot})/\pi$. The knots satisfy $\omega_{min}^2 \leq \omega_n'^{(L)} \leq \omega_{max}^2$ for all L, n and satisfy the same interlacing properties as the Gauss knots $\{\omega_n^{(L)}\}_{n=1}^L$ observed in Eq. (13). To the best of our knowledge, this is a new discretisation, which, unlike the Burkey-Cantrell discretisation, has not been probed numerically. We now state analogous theorems to that of Eq. (14), but with a smaller r.h.s. for otherwise unchanged parameters. We will make the distinction between when Hamiltonian Eq. (3) is massless and massive.

Theorem 2. *For any system observable $\hat{O}$, $\|\hat{O}\| < \infty$ the error introduced on it's expectation value at any time $t \geq 0$ when it's dynamics are approximated by the discretised Hamiltonian $\hat{H}'_L$, is bounded by*

1) *Massive case* ($\omega_{min} > 0$)

$$\begin{aligned} &\left|\mathrm{tr}\left[\hat{O}\mathrm{e}^{-\mathrm{i}t\hat{H}}\hat{\varrho}_0\mathrm{e}^{\mathrm{i}t\hat{H}}\right] - \mathrm{tr}\left[\hat{O}\mathrm{e}^{-\mathrm{i}t\hat{H}'_L}\hat{\varrho}_0\mathrm{e}^{\mathrm{i}t\hat{H}'_L}\right]\right|^2 \\ &\leq D_1\frac{(\omega_{max}t)^{2L+1}}{(2L+1)!}\left(\mathrm{e}^{\omega_{max}t}+1\right)\left(\|\vec{\gamma}'_0\|^{1/2} + \eta_1\|\hat{A}_{\mathcal{S}}\|t\right), \end{aligned} \tag{21}$$

2) *Massless case* ($\omega_{min} = 0$)

$$\begin{aligned} &\left|\mathrm{tr}\left[\hat{O}\mathrm{e}^{-\mathrm{i}t\hat{H}}\hat{\varrho}_0\mathrm{e}^{\mathrm{i}t\hat{H}}\right] - \mathrm{tr}\left[\hat{O}\mathrm{e}^{-\mathrm{i}t\hat{H}'_L}\hat{\varrho}_0\mathrm{e}^{\mathrm{i}t\hat{H}'_L}\right]\right|^2 \\ &\leq D_1\frac{(\omega_{max}t)^{2L+1}}{(2L+1)!}\left(\mathrm{e}^{\omega_{max}t}+1\right)\left(\|\vec{\gamma}'_0\|^{1/2} + \eta_1\|\hat{A}_{\mathcal{S}}\|\frac{\mathrm{e}^{\omega_{max}t}-1}{\omega_{max}}\right)\mathrm{e}^{\omega_{max}t} \end{aligned} \tag{22}$$

for $L = 1, 2, 3, \ldots$ where $D_1 = 4\eta_1\|\hat{O}\|^2\frac{\|\hat{A}_{\mathcal{S}}\|}{\omega_{max}}$, $\eta_1 = \sqrt{\frac{1}{\pi\omega_{max}}\int dx J(\sqrt{x})}$, and the operator $\vec{\gamma}'_0$ encodes information regarding 2-point correlation functions in $\mathcal{B}$ of the initial state. More precisely,

$$\vec{\gamma}'_0 = \begin{pmatrix} \vec{\gamma}'_{xx} & \vec{\gamma}'_{xp} \\ \vec{\gamma}'_{px} & \vec{\gamma}'_{pp} \end{pmatrix}, \tag{23}$$

where $[\vec{\gamma}'_{xx}]_{n,m} = \mathrm{tr}[\hat{x}'_n\hat{x}'_m\hat{\varrho}_0]$, $\left[\vec{\gamma}'_{xp}\right]_{n,m} = \mathrm{tr}[\hat{x}'_n\hat{p}'_m\hat{\varrho}_0]$, $\left[\vec{\gamma}'_{px}\right]_{n,m} = \mathrm{tr}[\hat{p}'_n\hat{x}'_m\hat{\varrho}_0]$, $\left[\vec{\gamma}'_{pp}\right]_{n,m} =$

$\mathrm{tr}[\hat{p}'_n\hat{p}'_m\hat{\varrho}_0]$, $n, m \in \mathbb{N}_+$ *with*

$$\begin{aligned}\hat{x}'_n &= \sqrt{\omega_{max}}\int \mu_0^{(1/2)}(dx)P'_{n-1}(x^2)\left(a_x^\dagger + a_x\right),\\ \hat{p}'_n &= \frac{\mathrm{i}}{\sqrt{\omega_{max}}}\int \mu_0^{(1/2)}(dx)P'_{n-1}(x^2)\,x\left(a_x^\dagger - a_x\right), \quad n \in \mathbb{N}_+\end{aligned} \tag{24}$$

on $\mathcal{B}$. Here $\hat{x}'_n$ and $\hat{p}'_n$ have been written in standard form (see section I).

See section VI A for proof. See section A 2 for alternative expressions for $\|\vec{\gamma}'_0\|$

Observations The bound that has been obtained in theorem 2 up to constant factors achieves the same error as the Burkey-Cantrell discretisation but with only half the number of knot points. This observation suggests an improved discretisation method using Gauss quadrature rules and may also find applications in analytical and numerical work.

Interestingly, for theorems (1) and (2) we used a Lieb-Robinson bound to derive a relation between two non-local Hamitonians (in Eq. (3) and its discretised counterparts Eqs. (11) and (19), every harmonic oscillator is coupled *directly* to the system via $\hat{A}_{\mathcal{S}}$). But now, in these non-local Hamiltonians, the notion of a distance that is normally associated with a lattice in the Lieb-Robinson bound plays the role of the number of Gauss knot points L.

Note also that for $\omega_{max} = \infty$, the upper bound in Eqs. (14) and (21) diverge. Under the minimal assumptions that have been made in this manuscript regarding the initial state $\hat{\varrho}_0$, this is to be expected since for $\omega_{max} = \infty$ we are sampling an unbounded interval with a finite number of sample points[42]. The theory of orthogonal polynomials also tells us that if the support of the spectral density is gapped, i.e. the spectral density vanishes strictly in an interval $[\omega_i, \omega_f]$ with $\omega_{min} < \omega_i < \omega_f < \omega_{max}$, a situation known to occur in physical systems such as photonic crystals[43], then the discretised bath will have at most one discrete mode in the gap $[\omega_i, \omega_f]$.

III. MULTIPLE BATHS EXTENSION

Often in physical settings, the quantum system on $\mathcal{S}$ is coupled to multiple continuous baths via different interaction terms. In such circumstances, the Hamiltonian is on $\mathcal{S} \otimes \mathcal{B}^{\otimes N}$ and reads

$$\hat{H}_{\text{mul}} = \hat{H}_{\mathcal{S}} \otimes \mathbb{1}_{\mathcal{B}}^{\otimes N} + \sum_{m=1}^{N} \hat{H}^{(m)}, \quad N \in \mathbb{N}_+ \tag{25}$$

where

$$\begin{aligned}\hat{H}^{(m)} =&\hat{A}_{\mathcal{S}}^{(m)} \otimes \mathbb{1}_{\mathcal{B}}^{\otimes m-1} \otimes \left(\int dk h^{(m)}(k)(a_k^{(m)\dagger} + a_k^{(m)}) \right) \otimes \mathbb{1}_{\mathcal{B}}^{\otimes N-m} \\ &+ \mathbb{1}_{\mathcal{S}} \otimes \mathbb{1}_{\mathcal{B}}^{\otimes m-1} \otimes \left(\int dk g^{(m)}(k) a_k^{(m)\dagger} a_k^{(m)} \right) \otimes \mathbb{1}_{\mathcal{B}}^{\otimes N-m}.\end{aligned} \tag{26}$$

Here each individual bath and interaction term $\hat{H}^{(m)}$ is defined as in Eq. (3) and will have its own spectral density $J^{(m)}$. Since they are independent bosonic baths, we also have $[a_x^{(n)}, a_y^{(m)\dagger}] = \delta_{n,m}\delta(x-y)$, $[a_x^{(n)}, a_y^{(m)}] = 0$. In analogy with Eqs. (11) and (19), we can define discretised versions of $\hat{H}^{(m)}$ according to the two discretisation schemes considered in this article. Similarly to Eq. (11), for Burkey-Cantrell discretisation, we define

$$\begin{aligned}\hat{H}_L^{(0,m)} =&\hat{A}_{\mathcal{S}}^{(m)} \otimes \mathbb{1}_{\mathcal{B}}^{\otimes m-1} \otimes \left(\sum_{n=1}^{L} h_n^{(m,L)}(c_n^{(m)\dagger} + c_n^{(m)}) \right) \otimes \mathbb{1}_{\mathcal{B}}^{\otimes N-m} \\ &+ \mathbb{1}_{\mathcal{S}} \otimes \mathbb{1}_{\mathcal{B}}^{\otimes m-1} \otimes \left(\sum_{n=1}^{L} \omega_n^{(m,L)} c_n^{(m)\dagger} c_n^{(m)} \right) \otimes \mathbb{1}_{\mathcal{B}}^{\otimes N-m}, \quad L, m \in \mathbb{N}_+\end{aligned} \tag{27}$$

where the Gauss knots $\omega_n^{(m,L)}$ and Gauss weights $(h_n^{(m,L)})^2$ are calculated from the weight function $J^{(m)}(\cdot)/\pi$, for which we denote its minimum and maximum frequencies by $\omega_{min}^{(m)}$ and $\omega_{max}^{(m)}$ respectively (see paragraph below Eq. (8)). Similarly to the second discretisation procedure we considered, Eq. (19), we define

$$\begin{aligned}\hat{H}_L^{(1,m)} =&\hat{A}_{\mathcal{S}}^{(m)} \otimes \mathbb{1}_{\mathcal{B}}^{\otimes m-1} \otimes \left(\sum_{n=1}^{L} \frac{h_n'^{(m,L)}}{\sqrt{2\bar{\omega}_n^{(m,L)}}} (c_n'^{(m)\dagger} + c_n'^{(m)}) \right) \otimes \mathbb{1}_{\mathcal{B}}^{\otimes N-m} \\ &+ \mathbb{1}_{\mathcal{S}} \otimes \mathbb{1}_{\mathcal{B}}^{\otimes m-1} \otimes \left(\sum_{n=1}^{L} \bar{\omega}_n^{(m,L)} c_n'^{(m)\dagger} c_n'^{(m)} \right) \otimes \mathbb{1}_{\mathcal{B}}^{\otimes N-m}, \quad L, m \in \mathbb{N}_+.\end{aligned} \tag{28}$$

We can now define the discretised Hamiltonian

$$\hat{H}_{\vec{L}}^{\vec{q}} = \hat{H}_{\mathcal{S}} \otimes \mathbb{1}_{\mathcal{B}}^{\otimes N} + \sum_{m=1}^{N} \hat{H}_{L_m}^{(q_m,m)}, \quad N \in \mathbb{N}_+ \tag{29}$$

where $\vec{q} = (q_1, q_2, \ldots, q_N)$ is a binary string and $\vec{L} = (L_1, L_2, \ldots, L_N)$. With the definitions

$$\left(\Delta_L^{(0,m)}(t)\right)^2 = D_0^{(m)} \frac{(\omega_{max}^{(m)} t)^{L+1}}{(L+1)!} \left(\mathrm{e}^{\omega_{max}^{(m)} t} + 1 \right) \left(\|\vec{\gamma}_0^{(m)}\|^{1/2} + \eta_0^{(m)} \|\hat{A}_{\mathcal{S}}\| t \right), \tag{30}$$

$$\left(\Delta_L^{(1,m)}(t)\right)^2 = \begin{cases} f_L^{(m)}(t) & \text{if } \omega_{min}^{(m)} > 0 \\ g_L^{(m)}(t) & \text{if } \omega_{min}^{(m)} = 0, \end{cases}$$

$$f_L^{(m)}(t) = C_1^{(m)} \frac{(\omega_{max}^{(m)} t)^{2L+1}}{(2L+1)!} (\mathrm{e}^{\omega_{max}^{(m)} t} + 1) \left(\|\vec{\gamma}_0^{(m)}\|^{1/2} + \eta_1^{(m)} \|\hat{A}_{\mathcal{S}}^{(m)}\| t \right)$$

$$g_L^{(m)}(t) = C_1^{(m)} \frac{(\omega_{max}^{(m)} t)^{2L+1}}{(2L+1)!} (\mathrm{e}^{2\omega_{max}^{(m)} t} + 1) \left(\|\vec{\gamma}_0^{(m)}\|^{1/2} + \eta_1^{(m)} (\mathrm{e}^{\omega_{max}^{(m)} t} - 1) \|\hat{A}_{\mathcal{S}}^{(m)}\| \right) \mathrm{e}^{\omega_{max}^{(m)} t} \tag{31}$$

$$\begin{aligned} D_0^{(m)} &= 8\eta_0^{(m)} \|\hat{O}\|^2 \|\hat{A}_{\mathcal{S}}^{(m)}\| / \omega_{max}^{(m)}, \quad \eta_0^{(m)} = \sqrt{\frac{2}{\pi} \int dx J^{(m)}(x)}, \\ C_1^{(m)} &= 4\eta_1^{(m)} \|\hat{O}\|^2 \|\hat{A}_{\mathcal{S}}^{(m)}\| / \omega_{max}^{(m)}, \quad \eta_1^{(m)} = \sqrt{\frac{1}{\pi \omega_{max}^{(m)}} \int dx J^{(m)}(\sqrt{x})}, \end{aligned} \tag{32}$$

where $\Delta_L^{(q,m)} \geq 0$, we have the following bounds.

Corollary 1. *For any system observable $\hat{O}$, $\|\hat{O}\| < \infty$ the error introduced on it's expectation value at any time $t \geq 0$ when it's dynamics are approximated by the discretised Hamiltonian $\hat{H}_{\vec{L}}^{\vec{q}}$, is bounded by*

$$\left| \mathrm{tr}\left[\hat{O} \mathrm{e}^{-\mathrm{i}t\hat{H}_{\text{mul}}} \hat{\varrho}_0 \mathrm{e}^{\mathrm{i}t\hat{H}_{\text{mul}}} \right] - \mathrm{tr}\left[\hat{O} \mathrm{e}^{-\mathrm{i}t\hat{H}_{\vec{L}}^{\vec{q}}} \hat{\varrho}_0 \mathrm{e}^{\mathrm{i}t\hat{H}_{\vec{L}}^{\vec{q}}} \right] \right| \leq \sum_{m=1}^{N} \Delta_{L_m}^{(q_m,m)}(t). \tag{33}$$

See section VI B for proof. We thus see that the error incurred scales linearly in the number of discretised continua.

IV. EXPLICIT EXAMPLES

For a range of spectral densities from the literature we will now present the explicit expressions for the frequencies and Gauss weights.

Consider the semi-circle law spectral density:

$$J(\omega) = C\sqrt{(\omega_{max} - \omega)(\omega - \omega_{min})}, \tag{34}$$

for some constant $C > 0$. This is the weight function of the Chebyshev polynomials of the second kind on the interval $[\omega_{min}, \omega_{max}]$. Their corresponding orthogonal polynomials and their zeros are known explicitly[38]. The zeros of the nth order Chebyshev polynomial on $[-1, 1]$ are

$$x_k = \cos\left(\frac{k}{n+1}\pi\right), \quad k = 1, \ldots, n \tag{35}$$

and hence for the Burkey-Cantrell discretisation (Eq. (11)), the discrete frequencies are

$$\omega_k^{(L)} = \frac{(\omega_{min} - \omega_{max})}{2} \cos\left(\frac{k}{L+1}\pi\right) + \frac{(\omega_{max} + \omega_{min})}{2}. \tag{36}$$

For the spectral density of the *Rubin model*[3] we find

$$J(\omega) = C\sqrt{(\omega_{max}^2 - \omega^2)(\omega^2 - \omega_{min}^2)}, \tag{37}$$

for some constant $C > 0$. From Eq. (55), we have that this corresponds to a Chebyshev weight function of the second kind for the measure $J(\sqrt{\cdot})/\pi$ used in Eq. (18). Thus we have for the 2nd discretisation method (Eq. (19))

$$\bar{\omega}_k^{(L)} = \sqrt{\frac{(\omega_{min}^2 - \omega_{max}^2)}{2} \cos\left(\frac{k}{L+1}\pi\right) + \frac{(\omega_{max}^2 + \omega_{min}^2)}{2}}. \tag{38}$$

Note that since the Chebyshev polynomials are known explicitly, we can also find explicitly the $h_n^{(L)}$ coefficients in both the above examples.

Now we will consider the frequently considered power-law spectral densities

$$J(\omega) = 2\pi\alpha(\omega_{max} - \omega_{min})(\omega - \omega_{min})^s, \quad -1 < s \tag{39}$$

which include the sub-ohmic $s < 1$, ohmic $s = 1$ and the super-ohmic $s > 1$ case. We can use the Jacobi Polynomials to describe the measures $J(\cdot)/\pi$ and $J(\sqrt{\cdot})/\pi$. For the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$ on $[-1, 1]$, we have the Buell inequalities for their zeros x_i ([44], pg 125):

$$\frac{i + (\alpha + \beta - 1)/2}{n + (\alpha + \beta + 1)/2}\pi < \nu_i < \frac{i}{n + (\alpha + \beta + 1)/2}\pi, \quad i = 1, \ldots, n \tag{40}$$

where $\nu_i = \arccos x_i$ and $-1/2 \leq \alpha \leq 1/2$, $-1/2 \leq \beta \leq 1/2$, excluding the case $\alpha^2 = \beta^2 = 1/4$. Hence for the Burkey-Cantrell discretisation (Eq. (11))

$$\begin{aligned} &\left[1 - \cos\left(\frac{k}{L + (s+1)/2}\pi\right)\right] \frac{\omega_{max} - \omega_{min}}{2} < \omega_k^{(L)} - \omega_{min} \\ &< \left[1 - \cos\left(\frac{k + (s-1)/2}{L + (s+1)/2}\pi\right)\right] \frac{\omega_{max} - \omega_{min}}{2} \end{aligned} \tag{41}$$

for $-1/2 \leq s \leq 1/2$. For the massless ($\omega_{min} = 0$) 2nd discretisation method (Eq. (19)),

$$\begin{aligned} &\omega_{max}\sqrt{\left[1 - \cos\left(\frac{k}{L + (s/2+1)/2}\pi\right)\right]/2} < \bar{\omega}_k^{(L)} \\ &< \omega_{max}\sqrt{\left[1 - \cos\left(\frac{k + (s/2-1)/2}{L + (s/2+1)/2}\pi\right)\right]/2} \end{aligned} \tag{42}$$

for $-1 < s \leq 1$. Note that other bounds for the zeros are known for the values of $-1 < s$ not covered here. See for example[45]. In all the examples in this section, the corresponding orthogonal polynomials are known explicitly and thus one can achieve explicit expressions for the Gauss weights too.

V. CONCLUSION

We derive two error bounds for dynamical observables when discretising a continuum of harmonic oscillators according to Gauss quadrature rules. For one of the bounds, numerical studies have probed this discretisation numerically in the past. For the second case, no prior numerical studies have been performed. The second bound achieves a sharper bound for the same parameters, suggesting that the second Gauss quadrature discretisation method may be more efficient.

To prove these results, we make use of a unitary mapping based on orthogonal polynomials and a Lieb-Robinson bound, providing yet another application to these powerful tools. Attempts to understand the errors endured by dynamical observables as a function of time when approximating a Hamiltonian with absolutely continuous spectrum with one of pure point spectrum, although receiving interest since 1929 by various authors, has up to now only consisted in numerical studies.

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VI. PROOFS

A. Proofs of theorems 1 and 2

For convenience, we will prove both theorems in parallel. The proof proceeds along three main steps. First, we will state unitary transformations of the bath modes which allow Eq. (3) to be written as a Hamiltonian in which the system on $\mathcal{S}$ couples to the first site of a nearest neighbour coupled harmonic chain. This chain is then truncated at finite length and a Lieb-Robinson bond is deployed to achieve error bounds for the expectation value of systems operators. Subsequently, the finite chain is transformed back to a non-local Hamiltonian and it is demonstrated that this achieves the discretised Hamiltonians as formulated in theorems 1 and 2.

In[37], it was shown that if $J(\cdot)$ has all moments finite, the Hamiltonian Eq. (3) can be written in the forms

$$\begin{aligned}\hat{H} =&\hat{H}_{\mathcal{S}} \otimes \mathbb{1}_{\mathcal{B}} + \sqrt{\beta_0(0)}\hat{A}_{\mathcal{S}} \otimes (b_0(0) + b_0^\dagger(0)) \\ &+ \mathbb{1}_{\mathcal{S}} \otimes \sum_{n=0}^{\infty} \alpha_n(0) b_n^\dagger(0) b_n(0) + \sqrt{\beta_{n+1}(0)}(b_{n+1}^\dagger(0) b_n(0) + h.c.)\end{aligned} \tag{43}$$

and

$$\begin{aligned}\hat{H} =&\hat{H}_{\mathcal{S}} \otimes \mathbb{1}_{\mathcal{B}} + \sqrt{\frac{\beta_0(1)}{\omega_{max}}}\hat{A}_{\mathcal{S}} \otimes \hat{X}_0 \\ &+ \mathbb{1}_{\mathcal{S}} \otimes \sum_{n=0}^{\infty} \left(\frac{\sqrt{\beta_{n+1}(1)}}{\omega_{max}} \hat{X}_n \hat{X}_{n+1} + \frac{\alpha_n(1)}{2\omega_{max}} \hat{X}_n^2 + \frac{\omega_{max}}{2} \hat{P}_n^2 \right) \\ &+ K \mathbb{1}_{\mathcal{S}} \otimes \mathbb{1}_{\mathcal{B}}.\end{aligned} \tag{44}$$

where

$$\hat{X}_n := \sqrt{\omega_{max}}\,(b_n^\dagger(1) + b_n(1)), \quad \hat{P}_n := \mathrm{i}(b_n^\dagger(1) - b_n(1))/(2\sqrt{\omega_{max}}), \quad n \in \mathbb{N}_0, \tag{45}$$

are position and momentum operators satisfying the canonical commutation relations. It was established in Theorem 33 of[37] that the operators $b_n(q), b_n^\dagger(q)$ are well defined on $\mathcal{D}(\mathfrak{n}^{1/2})$, where $\mathfrak{n} = d\hat{\Gamma}(\mathbb{1}_{\mathfrak{h}})$ is the second quantised boson number operator. $K \in \mathbb{R}$ thus w.l.o.g. from here on it will be set to zero since it does not contribute to Eq. (21). Now we will state a recently derived locality bound[31].

The Hamiltonian the bound applies to is system with Hamiltonian $\hat{H}_{\mathcal{S}}$ on $\mathcal{S}$ coupled to a semi-infinite nearest neighbour bosonic chain of the form

$$\hat{H}_{\mathcal{B}} = \frac{1}{2} \sum_{i,j=0}^{\infty} \left(\hat{x}_i X_{i,j} \hat{x}_j + \hat{p}_i P_{i,j} \hat{p}_j \right), \tag{46}$$

where $X_{i,j} = X_{j,i} \in \mathbb{R}$, $P_{i,j} = P_{j,i} \in \mathbb{R}$ where $X_{i,j} = P_{i,j} = 0$ for $|i-j| > 1$. The system-bath coupling is of the form $\hat{h} \otimes \hat{x}_0$, where $\hat{h}$ acts on the system and is bounded in operator norm. The total Hamiltonian reads

$$\hat{H} = \hat{H}_{\mathcal{S}} \otimes \mathbb{1}_{\mathcal{B}} + \hat{h} \otimes \hat{x}_0 + \mathbb{1}_{\mathcal{S}} \otimes \hat{H}_{\mathcal{B}}. \tag{47}$$

We then define a spatially truncated Hamiltonian

$$\begin{aligned}\hat{H}_L &= \hat{H}_{\mathcal{S}} \otimes \mathbb{1}_{\mathcal{B}} + \hat{h} \otimes \hat{x}_0 + \mathbb{1}_{\mathcal{S}} \otimes \hat{H}_{\mathcal{B}}^L, \\ \hat{H}_{\mathcal{B}}^L &= \frac{1}{2} \sum_{i,j=0}^{L-1} \left(\hat{x}_i X_{i,j} \hat{x}_j + \hat{p}_i P_{i,j} \hat{p}_j \right)\end{aligned} \tag{48}$$

and the constant c such that $\|X_L P_L\|^{1/2} \leq c$. Theorem 1 in[31] for $X, P > 0$ or $X = P$ gives us the bound

$$\frac{\left|\mathrm{tr}\left[\hat{O}\mathrm{e}^{-\mathrm{i}\hat{H}t}\hat{\varrho}_0\mathrm{e}^{\mathrm{i}\hat{H}t}\right] - \mathrm{tr}\left[\hat{O}\mathrm{e}^{-\mathrm{i}\hat{H}_L t}\hat{\varrho}_0\mathrm{e}^{\mathrm{i}\hat{H}_L t}\right]\right|^2}{4\|\hat{O}\|^2\|\hat{h}\|/c} \leq \frac{C(\|\vec{\gamma}_0\|^{\frac{1}{2}} + \|\hat{h}\|t)(ct)^{L+1}(\mathrm{e}^{ct}+1)}{(L+1)!}, \tag{49}$$

where

$$C = \|P_L\||X_{L-1,L}|/c^2 + |P_{L-1,L}|/c \tag{50}$$

and

$$\vec{\gamma}_0 = \begin{pmatrix} \vec{\gamma}_{xx} & \vec{\gamma}_{xp} \\ \vec{\gamma}_{px} & \vec{\gamma}_{pp} \end{pmatrix}, \quad [\vec{\gamma}_{ab}]_{i,j} = \mathrm{tr}[\hat{a}_i \hat{b}_j \hat{\varrho}_0], \quad a, b = x, p, \tag{51}$$

collects the two-point bath correlations in the initial state. Also note that $|X_{L-1,L}| \leq \|X_L\| \leq \|X\|$ and $|P_{L-1,L}| \leq \|P_L\| \leq \|P\|$. If $X, P > 0$ or $X = P$ are not satisfied, we use theorem 3 in[31] to achieve the bound. Let c' such that $\{\|X\|, \|P\|\} \leq c'$, then for all X, P

$$\begin{aligned} &\frac{\left|\mathrm{tr}\left[\hat{O}\mathrm{e}^{-\mathrm{i}\hat{H}t}\hat{\varrho}_0\mathrm{e}^{\mathrm{i}\hat{H}t}\right] - \mathrm{tr}\left[\hat{O}\mathrm{e}^{-\mathrm{i}\hat{H}_L t}\hat{\varrho}_0\mathrm{e}^{\mathrm{i}\hat{H}_L t}\right]\right|^2}{4\|\hat{O}\|^2\|\hat{h}\|/c} \\ &\qquad \leq \frac{C\mathrm{e}^{c't}(\|\vec{\gamma}_0\|^{1/2} + \|\hat{h}\|\frac{\mathrm{e}^{c't}-1}{c'})(ct)^{L+1}(\mathrm{e}^{ct}+1)}{(L+1)!}. \end{aligned} \tag{52}$$

If $P \propto \mathbb{1}$, we may replace the factor $(ct)^{L+1}/(L+1)!$ by $(ct)^{2L+1}/(2L+1)!$ in the R.H.S. of Eqs. (49), (52). We can readily apply these bounds to Eqs. (43) and (44). First define position and momentum operators

$$\hat{x}_n(0) := (b_n^\dagger(0) + b_n(0))/\sqrt{2}, \quad \hat{p}_n(0) := \mathrm{i}(b_n^\dagger(0) - b_n(0))/\sqrt{2}, \quad n \in \mathbb{N}_0. \tag{53}$$

Comparing Eq. (46) with Eqs. (43), (44) and the definition of the Jacobi matrices $\mathcal{J}(d\lambda^q)$ (see Eq. (162) in[37]), we find[46]

For Eq. (43):

$$X = P = \mathcal{J}(d\lambda^0), \quad \hat{h} = \sqrt{2\beta_0(0)}\hat{A}_{\mathcal{S}}, \quad d\lambda^0(x) = \pi^{-1}J(x)dx. \tag{54}$$

For Eq. (44):

$$X = \frac{\mathcal{J}(d\lambda^1)}{\omega_{max}}, \quad P = \mathbb{1}\,\omega_{max}, \quad \hat{h} = \sqrt{\frac{\beta_0(1)}{\omega_{max}}}\hat{A}_{\mathcal{S}}, \quad d\lambda^1(x) = \pi^{-1}J(\sqrt{x})dx. \tag{55}$$

From Eqs (15,156,160) in[37],

$$\beta_0(0) = \int dx J(x)/\pi, \quad \beta_0(1) = \int dx J(\sqrt{x})/\pi. \tag{56}$$

Since the spectrum of a Jacobi matrix is equal to its minimally closed support interval[47], we have for the Eqs. (43), (44): $\|X\| = \|P\| = \sqrt{\|XP\|} = \omega_{max}$, and $X > 0$ iff $\omega_{min} > 0$. The r.h.s. of Eqs. (14), (21) and (22) are a direct consequence of these bounds. We will now proceed to apply another unitary transformation. This time, we will apply it to the above spatially truncated Hamiltonians to write them in terms of Gauss quadrature.

Both Eqs. (43) and (44) can be written in the compact form (see Eq. (162) in[37])

$$\begin{aligned} H =& \hat{H}_S \otimes \mathbb{1}_{\mathcal{B}} + \sqrt{\beta_0(q)}\, \hat{A}_{\mathcal{S}} \otimes (b^\dagger(q) + b(q)) \\ &+ \mathbb{1}_{\mathcal{S}} \otimes \frac{q}{2} \left[\vec{b}^\top(q) \left(\mathcal{J}(d\lambda^q) - \frac{q}{4}\mathbb{1} \right) \vec{b}(q) + h.c. \right] \\ &+ \mathbb{1}_{\mathcal{S}} \otimes \vec{b}^\dagger(q) \left(\mathcal{J}(d\lambda^q) + \frac{q}{4}\mathbb{1} \right) \vec{b}(q), \end{aligned} \tag{57}$$

where

$$\begin{aligned} \vec{b}^\dagger(q) &:= (b_0^\dagger(q), b_1^\dagger(q), b_2^\dagger(q), b_3^\dagger(q), \ldots), \\ \vec{b}(q) &:= (b_0(q), b_1(q), b_2(q), b_3(q), \ldots)^\top, \end{aligned} \tag{58}$$

and Eq. (43) is given when $q = 0$ while Eq. (44) when $q = 1$. In the case of the truncated chains $\hat{H}_L$and $\hat{H}'_L$, we simply replace $\mathcal{J}$ with $\mathcal{J}_L := \mathcal{J}_{[1:L;1:L]}$, $\mathbb{1}$ with $\mathbb{1}_{[1:L;1:L]}$ and $\vec{b}$ with $\vec{b}_{[1:L]}$. Since Jacobi matrices are real symmetric, they are diagonalisable via an orthogonal transformation. Thus

$$\mathcal{J}_L(d\lambda^q) = O_L(d\lambda^q) D^{(L)}(d\lambda^q) O_L^\top(d\lambda^q) \tag{59}$$

where $\mathrm{diag} D^{(L)}(d\lambda^q) = (\omega_1^{(L)}(d\lambda^q), \ldots, \omega_L^{(L)}(d\lambda^q))$ are the eigenvalues of $\mathcal{J}(d\lambda^q)$ and $O_L(d\lambda^q) = (\vec{v}_1(d\lambda^q), \ldots, \vec{v}_L(d\lambda^q))$ with $\vec{v}_i(d\lambda^q)$ the normalised eigenvector for $\omega_i^{(L)}(d\lambda^q)$. Let $\tilde{P}_n(d\lambda^q, x)$ be the real orthogonal polynomial of order n corresponding to the measure $d\lambda^q(x)$:

$$\int d\lambda^q(x) \tilde{P}_n(d\lambda^q; x) \tilde{P}_m(d\lambda^q; x) = ||\tilde{P}_n||^2_{d\lambda^q}\, \delta_{m,n}, \quad n, m \in \mathbb{N}_0 \tag{60}$$

where $m = n$ defines $||\tilde{P}_n||_{d\lambda^q}$. The set $\{\tilde{P}_n(x; d\lambda^q)\}_{n=0}^\infty$ exists and for a specific choice of normalisation $\{||\tilde{P}_n||_{d\lambda^q}\}_{n=0}^\infty$, it is unique up to a real phase[38]. It is known that $\{\omega_i^{(j)}(d\lambda^q) \in \mathbb{R}\}_{i=1}^j$ are the zeros of $\tilde{P}_j(d\lambda^q; x)$ and

$$\begin{aligned} &\vec{v}_i(d\lambda^q) = \\ &\vec{(}\tilde{P}_0(d\lambda^q, \omega_i^{(L)}(d\lambda^q)), \ldots, \tilde{P}_{L-1}(d\lambda^q, \omega_i^{(L)}(d\lambda^q)))^\top \frac{1}{\sqrt{\sum_{k=0}^{L-1} \tilde{P}_k^2(d\lambda^q; \omega_i^{(L)}(d\lambda^q))}} \end{aligned} \tag{61}$$

[38]. Let us define

$$h_j^{(L)}(d\lambda^q) := \frac{\sqrt{\beta_0(d\lambda^q)}\tilde{P}_0(d\lambda^q;\omega_j^{(L)}(d\lambda^q))}{\sqrt{\sum_{k=0}^{L-1}\tilde{P}_k^2(d\lambda^q;\omega_j^{(L)}(d\lambda^q))}}, \quad j\in\mathbb{N}_+. \tag{62}$$

Hence for Eq. (43):

$$\hat{H}_L = \hat{H}_{\mathcal{S}}\otimes\mathbb{1}_{\mathcal{B}} + \hat{A}_{\mathcal{S}}\otimes\sum_{n=1}^{L} h_n^{(L)}(d\lambda^0)(c_n^\dagger + c_n) + \mathbb{1}_{\mathcal{S}}\otimes\sum_{n=1}^{L}\omega_n^{(L)}(d\lambda^0)c_n^\dagger c_n \tag{63}$$

where $\vec{c} := O_L^\top(d\lambda^0)\vec{b}(0)_{[1:L]}$, $\vec{c}^\dagger := \vec{b}^\dagger(0)_{[1:L]}O_L(d\lambda^0)$. We can easily verify that $[c_i, c_j^\dagger] = \delta_{i,j}$, $[c_i, c_j] = 0$ and are hence bosonic creation annihilation operators. If we use orthonormal polynomials (i.e. $||\tilde{P}_n||_{d\lambda^q} = 1$), then the zeroth order polynomial is $\tilde{P}_0(d\lambda^q;x) = 1/\sqrt{\beta_0(q)}$ and hence we find the results stated in theorem 1. For Eq. (44), we have

$$\hat{H}_L = \hat{H}_{\mathcal{S}}\otimes\mathbb{1}_{\mathcal{B}} + \hat{A}_{\mathcal{S}}\otimes\sum_{n=1}^{L}\frac{h_n^{(L)}(d\lambda^1)}{\sqrt{2\bar{\omega}_n^{(L)}}}(c_n'^\dagger + c_n') + \mathbb{1}_{\mathcal{S}}\otimes\sum_{n=1}^{L}\bar{\omega}_n^{(L)}c_n'^\dagger c_n' \tag{64}$$

where $\bar{\omega}_n^{(L)} := \sqrt{\omega_n^{(L)}(d\lambda^1)}$,

$$\begin{aligned} c_n' :=& \sqrt{\frac{\bar{\omega}_n^{(L)}}{2}}\Bigg[\left(1+\frac{1}{2\bar{\omega}_n^{(L)}}\right)\left[O_L^\top(d\lambda^1)\vec{b}(1)_{[1:L]}\right]_n \\ &+ \left(1-\frac{1}{2\bar{\omega}_n^{(L)}}\right)\left[\vec{b}^\dagger(1)_{[1:L]}O_L(d\lambda^1)\right]_n\Bigg] \end{aligned} \tag{65}$$

$$\begin{aligned} c_n'^\dagger :=& \sqrt{\frac{\bar{\omega}_n^{(L)}}{2}}\Bigg[\left(1+\frac{1}{2\bar{\omega}_n^{(L)}}\right)\left[\vec{b}^\dagger(1)_{[1:L]}O_L(d\lambda^1)\right]_n \\ &+ \left(1-\frac{1}{2\bar{\omega}_n^{(L)}}\right)\left[O_L^\top(d\lambda^1)\vec{b}(1)_{[1:L]}\right]_n\Bigg] \end{aligned} \tag{66}$$

with $[c_i', c_j'^\dagger] = \delta_{i,j}$, $[c_i', c_j'] = 0$ thus achieving the results of theorem 2. From the theory of orthogonal polynomials[38], it is also known that $\omega_n^{(L)}(d\lambda^q)$ are contained in the support interval of $d\lambda^q$ and that the zeros of $P_n(d\lambda^q;x)$ alternate with those of $P_{n+1}(d\lambda^q;x)$, that is

$$\begin{aligned} &\omega_{n+1}^{(n+1)}(d\lambda^q) < \omega_n^{(n)}(d\lambda^q) < \omega_n^{(n+1)}(d\lambda^q) < \omega_{n-1}^{(n)}(d\lambda^q) < \ldots \\ &< \omega_1^{(n)}(d\lambda^q) < \omega_1^{(n+1)}(d\lambda^q) \end{aligned} \tag{67}$$

where $\omega_i^{(n+1)}$, and $\omega_j^{(n)}$ are ordered in descending order.

Using Eqs. (158) and (161) in[37], we can establish the relation between the field operators $a(f) = \int dx f(x) a_x$, $a^\dagger(f) = \int dx f(x) a_x^\dagger$ in Eq. (3) and the operators $c_n, c_n^\dagger, c'_n, c'^\dagger_n$.

$$\begin{aligned} c_n &= \sum_{j=0}^{L-1} \frac{\tilde{P}_j(d\lambda^0; \omega_n^{(L)}(d\lambda^0))}{\sqrt{\sum_{k=0}^{L-1} \tilde{P}_k^2(d\lambda^0; \omega_n^{(L)}(d\lambda^0))}}\, a(\vec{\gamma}_n^0), \\ c_n^\dagger &= \sum_{j=0}^{L-1} \frac{\tilde{P}_j(d\lambda^0; \omega_n^{(L)}(d\lambda^0))}{\sqrt{\sum_{k=0}^{L-1} \tilde{P}_k^2(d\lambda^0; \omega_n^{(L)}(d\lambda^0))}}\, a^\dagger(\vec{\gamma}_n^0), \end{aligned} \tag{68}$$

$$\begin{aligned} c'_n &= \sqrt{\frac{\bar{\omega}_n^{(L)}}{2}} \left(\sum_{j=0}^{L-1} \frac{\tilde{P}_j(d\lambda^1; \omega_n^{(L)}(d\lambda^1))}{\sqrt{\sum_{k=0}^{L-1} \tilde{P}_k^2(d\lambda^1; \omega_n^{(L)}(d\lambda^1))}} \left(a^\dagger(f_j^n) + a(g_j^n) \right) \right), \\ c'^\dagger_n &= \sqrt{\frac{\bar{\omega}_n^{(L)}}{2}} \left(\sum_{j=0}^{L-1} \frac{\tilde{P}_j(d\lambda^1; \omega_n^{(L)}(d\lambda^1))}{\sqrt{\sum_{k=0}^{L-1} \tilde{P}_k^2(d\lambda^1; \omega_n^{(L)}(d\lambda^1))}} \left(a(f_j^n) + a^\dagger(g_j^n) \right) \right), \end{aligned} \tag{69}$$

where $f_j^n(x) := \gamma_j^1(x)(1 + g(x)/\bar{\omega}_n^{(L)})$, $g_j^n(x) := \gamma_j^1(x)(1 - g(x)/\bar{\omega}_n^{(L)})$. If $x \in \mathbb{R}$,

$$\gamma_n^q(x) := P_n(d\lambda^q; g^{q+1}(x)) \sqrt{\frac{J(g^{q+1}(x))}{\pi} \left| \frac{dg(x)}{dx} \right|}, \tag{70}$$

and can be generalised for higher dimensions by writing Hamiltonian Eq. (3) in *standard form* (see section I). We now turn our attention to $\vec{\gamma}_0$. We start with deriving its value for the case of theorem 1. From Eqs. (51), (43) and recalling the definitions (53), we find[48] $[\vec{\gamma}_{xx}]_{i,j} = \mathrm{tr}[\hat{x}_{i-1}(0)\hat{x}_{j-1}(0)\hat{\varrho}_0]$, $[\vec{\gamma}_{xp}]_{i,j} = \mathrm{tr}[\hat{x}_{i-1}(0)\hat{p}_{j-1}(0)\hat{\varrho}_0]$, $[\vec{\gamma}_{px}]_{i,j} = \mathrm{tr}[\hat{p}_{i-1}(0)\hat{x}_{j-1}(0)\hat{\varrho}_0]$, $[\vec{\gamma}_{pp}]_{i,j} = \mathrm{tr}[\hat{p}_{i-1}(0)\hat{p}_{j-1}(0)\hat{\varrho}_0]$, $i, j \in \mathbb{N}_+$. From Eq. (160-161) in[37] we have that

$$\begin{aligned} \hat{x}_n(0) &= \int \mu_0^{(1/2)}(dx) P_n(x)(a_x^\dagger + a_x), \\ \hat{p}_n(0) &= \mathrm{i} \int \mu_0^{(1/2)}(dx) P_n(x)(a_x^\dagger - a_x), \quad n \in \mathbb{N}_0, \end{aligned} \tag{71}$$

thus achieving Eqs. (15), (16) in theorem 1. We achieve the expression for $\|\vec{\gamma}'_0\|$ in theorem 2 similarly. Namely, from Eq. (45) and Eq. (158) in[37], we find

$$\begin{aligned} \hat{X}'_n &= \sqrt{\omega_{max}} \int \mu_0^{(1/2)}(dx) P'_n(x^2) \left(a_x^\dagger + a_x \right), \\ \hat{P}'_n &= \frac{\mathrm{i}}{\sqrt{\omega_{max}}} \int \mu_0^{(1/2)}(dx) P'_n(x^2)\, x \left(a_x^\dagger - a_x \right), \quad n \in \mathbb{N}_0 \end{aligned} \tag{72}$$

thus after the definitions $\hat{x}'_n := \hat{X}_{n-1}$, $\hat{p}'_n := \hat{P}_{n-1}$, $n \in \mathbb{N}_+$ we achieve Eqs. (23), (24) in theorem 2. □

B. Multiple chains extension proof

Here we will prove corollary 1. Let

$$G^{(L_1,L_2,\ldots,L_N)} = \mathrm{tr}\big[\hat{O}\mathrm{e}^{-\mathrm{i}t\hat{H}^{\vec{q}}_{\vec{L}}}\hat{\varrho}_0\mathrm{e}^{\mathrm{i}t\hat{H}^{\vec{q}}_{\vec{L}}}\big] \tag{73}$$

where we will denote the scenario that the nth bath has not been discretised, by replacing L_n by ∞. We now add and subtract G $N-1$ times to the r.h.s. of Eq. (33) each time discretising one more bath and starting with only one bath discretised. We then apply the triangle inequality and arrive at

$$\begin{aligned}
&\Big|\mathrm{tr}\big[\hat{O}\mathrm{e}^{-\mathrm{i}t\hat{H}_{\mathrm{mul}}}\hat{\varrho}_0\mathrm{e}^{\mathrm{i}t\hat{H}_{\mathrm{mul}}}\big] - \mathrm{tr}\big[\hat{O}\mathrm{e}^{-\mathrm{i}t\hat{H}^{\vec{q}}_{\vec{L}}}\hat{\varrho}_0\mathrm{e}^{\mathrm{i}t\hat{H}^{\vec{q}}_{\vec{L}}}\big]\Big| \\
&\leq \left|G^{(\infty,\ldots,\infty,\infty)} - G^{(\infty,\ldots,\infty,L_N)}\right| + \left|G^{(\infty,\ldots,\infty,L_N)} - G^{(\infty,\ldots,\infty,L_{N-1},L_N)}\right| \\
&\quad + \ldots + \left|G^{(\infty,L_2,L_3,\ldots,L_N)} - G^{(L_1,L_2,L_3,\ldots,L_N)}\right|.
\end{aligned} \tag{74}$$

In every pair on the r.h.s. of the inequality, there is always one bath which is discretised in one of the G terms but is not discretised for the other G term. We can thus define all the other baths to be part of the system Hamiltonian and then apply theorem 1 or theorem 2 to it. This gives us Eq. (33). □

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Appendix A: Appendix: Alternative expressions for $\|\vec{\gamma}_0\|$, $\|\vec{\gamma}_0'\|$ and examples

In this appendix we derive alternative expressions for the constants $\|\vec{\gamma}_0\|$, $\|\vec{\gamma}_0'\|$ which appear in theorems 1 and 2 respectively. These alternative expressions come in the form of Eqs. (A12) and (A32) respectively. In addition, we calculate explicitly $\|\vec{\gamma}_0\|$, $\|\vec{\gamma}_0'\|$ for some examples cases of particular initial quantum states $\hat{\varrho}_0 \in \mathcal{S} \otimes \mathcal{B}$; see sections A 1 c, and A 2 c respectively. We start with $\|\vec{\gamma}_0\|$.

1. Alternative expressions for $\|\vec{\gamma}_0\|$

Recall that the measure $\mu_0(dx) = \pi^{-1}J(x)dx$ is determinate, and thus $\{P_k\}_{k=0}^{\infty}$ form a complete orthonormal system in $L^2(\mu_0(dx))$ (see[50],[51]). Hence Eq. 16 represents an expansion of

$$\begin{aligned}\hat{x}(f) &:= \frac{1}{\sqrt{2}}\int \mu_0^{(1/2)}(dx) f(x)\left(a_x^\dagger + a_x\right),\\ \hat{p}(f) &:= \frac{\mathrm{i}}{\sqrt{2}}\int \mu_0^{(1/2)}(dx) f(x)\left(a_x^\dagger - a_x\right),\end{aligned} \tag{A1}$$

where $f \in L^2(\mu_0(dx))$ and recall $\mu_0^{(1/2)}(dx) := \sqrt{J(x)/\pi}\,dx$. Namely,

$$\begin{aligned}\hat{x}(f) &= \sum_{n=1}^{\infty} c_n(f)\hat{x}_n,\\ \hat{p}(f) &= \sum_{n=1}^{\infty} c_n(f)\hat{p}_n, \quad c_n \in \mathbb{R}.\end{aligned} \tag{A2}$$

a. Basis invariance of $\|\vec{\gamma}_0\|$

One can perform any unitary transformation of the operators $\{\hat{x}_n, \hat{p}_n\}_{n=1}^{\infty}$ into a new set $\{\underline{\hat{x}}_n, \underline{\hat{p}}_n\}_{n=1}^{\infty}$ with relationship $\vec{R} = \vec{U}\underline{\vec{R}}$, $\vec{U}^\dagger\vec{U} = \vec{U}\vec{U}^\dagger = \vec{\mathbb{1}}$, $\vec{R} := (\hat{x}_1, \hat{x}_2, \ldots, \hat{p}_1, \hat{p}_2, \ldots)^\top$, $\underline{\vec{R}} := (\underline{\hat{x}}_1, \underline{\hat{x}}_2, \ldots, \underline{\hat{p}}_1, \underline{\hat{p}}_2, \ldots)^\top$. Similarly to before we can define

$$\underline{\vec{\gamma}}_0 = \begin{pmatrix} \underline{\vec{\gamma}}_{xx} & \underline{\vec{\gamma}}_{xp} \\ \underline{\vec{\gamma}}_{px} & \underline{\vec{\gamma}}_{pp} \end{pmatrix}, \tag{A3}$$

where $\left[\underline{\vec{\gamma}}_{xx}\right]_{n,m} = \mathrm{tr}[\underline{\hat{x}}_n\underline{\hat{x}}_m\hat{\varrho}_0]$, $\left[\underline{\vec{\gamma}}_{xp}\right]_{n,m} = \mathrm{tr}[\underline{\hat{x}}_n\underline{\hat{p}}_m\hat{\varrho}_0]$, $\left[\underline{\vec{\gamma}}_{px}\right]_{n,m} = \mathrm{tr}[\underline{\hat{p}}_n\underline{\hat{x}}_m\hat{\varrho}_0]$, $\left[\underline{\vec{\gamma}}_{pp}\right]_{n,m} = \mathrm{tr}[\underline{\hat{p}}_n\underline{\hat{p}}_m\hat{\varrho}_0]$ for $n, m \in \mathbb{N}_+$. It immediately follows by direct substitution $\vec{\gamma}_0 = \vec{U}\underline{\vec{\gamma}_0}\vec{U}^\dagger$ and thus

$$\|\vec{\gamma}_0\| = \|\underline{\vec{\gamma}_0}\|. \tag{A4}$$

Eq. (A4) shows that the two-point correlation functions can be provided in any unitarily equivalent basis. Indeed, we now show that this feature allows us to write $\|\vec{\gamma}_0\|$ in a particularly appealing form.

b. Alternative expression for $\|\vec{\gamma}_0\|$

Denoting the complex conjugation by $(\cdot)^*$, we have $(\mathrm{tr}[\hat{x}_n\hat{p}_m\hat{\varrho}_0])^* = \mathrm{tr}[(\hat{x}_n\hat{p}_m\hat{\varrho}_0)^\dagger] = \mathrm{tr}[\hat{p}_m\hat{x}_n\hat{\varrho}_0]$ $\forall\, n, m \in \mathbb{N}_+$, where we have used the invariance of the trace under cyclic permutations and the

self-adjointness of $\hat{x}_n$, $\hat{p}_n$, $\hat{\varrho}_0$. We thus find

$$\vec{\gamma}_0^\dagger = \begin{pmatrix} \vec{\gamma}_{xx} & \vec{\gamma}_{xp} \\ \vec{\gamma}_{px} & \vec{\gamma}_{pp} \end{pmatrix}^\dagger = \begin{pmatrix} \vec{\gamma}_{xx}^\dagger & \vec{\gamma}_{px}^\dagger \\ \vec{\gamma}_{xp}^\dagger & \vec{\gamma}_{pp}^\dagger \end{pmatrix} = \vec{\gamma}_0. \tag{A5}$$

From Eq. (A5) we see that $\vec{\gamma}_0$ is self-adjoint and hence its operator norm takes on the form

$$\|\vec{\gamma}_0\| = \sup_{\|\vec{v}\|=1} \langle \vec{\gamma}_0 \vec{v}, \vec{v} \rangle, \tag{A6}$$

where $\langle \vec{\gamma}_0 \vec{v}, \vec{v} \rangle = \vec{x}^\top \vec{\gamma}_{xx} \vec{x} + \vec{p}^\top \vec{\gamma}_{px} \vec{x} + \vec{x}^\top \vec{\gamma}_{xp} \vec{p} + \vec{p}^\top \vec{\gamma}_{pp} \vec{p}$, with $\vec{v} = \vec{x} \oplus \vec{p} \in \mathbb{R}^\infty$. Using (16) and the linearity of the trace, we can write this as

$$\begin{aligned} \langle \vec{\gamma}_0 \vec{v}, \vec{v} \rangle = & \operatorname{tr}[\hat{x}(f_{\vec{x}})\, \hat{x}(f_{\vec{x}}) \hat{\varrho}_0] + \operatorname{tr}[\hat{p}(f_{\vec{p}})\, \hat{x}(f_{\vec{x}}) \hat{\varrho}_0] \\ & + \operatorname{tr}[\hat{x}(f_{\vec{x}})\, \hat{p}(f_{\vec{p}}) \hat{\varrho}_0] + \operatorname{tr}[\hat{p}(f_{\vec{p}})\, \hat{p}(f_{\vec{p}}) \hat{\varrho}_0], \end{aligned} \tag{A7}$$

where we have used the notation of Eq. (A1) and defined

$$f_{\vec{z}} = f_{\vec{z}}(x) = \sum_{k=1}^{\infty} P_{k-1}(x) z_k, \quad \vec{z} = \vec{x}, \vec{p}. \tag{A8}$$

Since $\{P_k\}_{k=0}^\infty$ form a complete orthonormal system, for every function $g \in L^2(\mu_0(dx))$ we can associate uniquely (once a sign convention for the set $\{P_k\}_{k=0}^\infty$ has been chosen) a vector $\vec{g} \in \mathbb{N}^\infty$. This is achieved by writing g in the form

$$g(x) = \sum_{k=1}^{\infty} g_k P_{k-1}(x). \tag{A9}$$

Let us define the set of functions in $L^2(\mu_0(dx))$ with a specific normalization,

$$L^2_{\text{nor}}(\mu_0(dx), E) := \left\{ f \in L^2(\mu_0(dx)) \;\middle|\; \int \mu_0(dx) f^2(x) = E \right\}. \tag{A10}$$

Writing a function $g \in L^2(\mu_0(dx))$ in terms of its associated vector $\vec{g}$, using Eq. (A9) we achieve

$$\int \mu_0(dx) g^2(x) = \sum_{m,n=1}^{\infty} g_m g_n \int \mu_0(dx) P_{m-1}(x) P_{n-1}(x) = \sum_{n=1}^{\infty} g_n^2 = \|\vec{g}\|^2. \tag{A11}$$

Thus a function $g \in L^2(\mu_0(dx))$ is in $L^2_{\text{nor}}(\mu_0(dx), E)$ iff its associated vector $\vec{g}$ satisfies $\|\vec{g}\|^2 = E$. Hence noting that $\|\vec{v}\|^2 = \|\vec{x}\|^2 + \|\vec{p}\|^2$, from Eqs. (A6), (A7), (A8) we conclude

$$\begin{aligned} \|\vec{\gamma}_0\| = \sup_{\substack{f_1 \in L^2_{\text{nor}}(\mu_0(dx), E), \\ f_2 \in L^2_{\text{nor}}(\mu_0(dx), 1-E), \\ E \in [0,1]}} & \Big(\operatorname{tr}[\hat{x}(f_1)\, \hat{x}(f_1) \hat{\varrho}_0] + \operatorname{tr}[\hat{p}(f_2)\, \hat{x}(f_1) \hat{\varrho}_0] \\ & + \operatorname{tr}[\hat{x}(f_1)\, \hat{p}(f_2) \hat{\varrho}_0] + \operatorname{tr}[\hat{p}(f_2)\, \hat{p}(f_2) \hat{\varrho}_0] \Big). \end{aligned} \tag{A12}$$

Eq. (A12) represents an alternative method to calculate $\|\vec{\gamma}_0\|$ in which one has to take the supremum over functions f_1, f_2.

c. Examples for $\|\vec{\gamma}_0\|$

Since the operators $\hat{x}_n$, $\hat{p}_n$ in Eq. (16) only act non trivially on the bath $\mathcal{B}$, one only needs to specify $\hat{\varrho}_{\rm B} := \mathrm{tr}_{\mathcal{S}}[\hat{\varrho}_0]$ (rather than the full initial quantum state $\hat{\varrho}_0$ on $\mathcal{S}\otimes\mathcal{B}$) in order to calculate $\|\vec{\gamma}_0\|$. For the interest of finding a simple example, it is useful to write $\hat{\varrho}_{\rm B}$ the terms of the local number basis of the raising and lowering operators $b_n^\dagger(0), b_n(0)$ defined in section VI. This basis was first introduced on page 165 of[37], and forms a complete basis for quantum states on $\mathcal{B}$. For every $n \in \mathbb{N}_0$, its associated number basis is generated by the usual relations $b_n(0)|0\rangle_n = 0$, $b_n^\dagger(0)|m\rangle_n = \sqrt{m+1}|m+1\rangle_n$. For our example, we will focus on the special case where there are n_0 excitation's in each oscillator. The state is then

$$\hat{\varrho}_{\rm B} = \hat{\rho}_0 \otimes \hat{\rho}_1 \otimes \hat{\rho}_2 \ldots, \tag{A13}$$

where $\hat{\rho}_n = |n_0\rangle_n\langle n_0|,\ n \in \mathbb{N}_0$. For $\hat{\varrho}_{\rm B}$ in Eq. (A13), Eq. (15) takes the form,

$$\vec{\gamma}_0 = \begin{pmatrix} (n_0+1/2)\mathbb{1} & (\mathrm{i}/2)\mathbb{1} \\ (-\mathrm{i}/2)\mathbb{1} & (n_0+1/2)\mathbb{1} \end{pmatrix}, \tag{A14}$$

where the $\vec{\gamma}_0$ has been written in the same block form as in Eq. (15). Eq. (A14) has two degenerate eigenvalues, namely n_0 and n_0+1. Thus

$$\|\vec{\gamma}_0\| = n_0 + 1. \tag{A15}$$

A particular physically transparent case of Eq. (A15), is when $n_0 = 0$. For this choice, $\hat{\varrho}_{\rm B}$ is the vacuum state of the bath Hamiltonian $d\hat{\Gamma}(G)$. Indeed, as pointed out in[37], the vacuum state of $d\hat{\Gamma}(G)$ is the same vacuum state as that defined by the number basis of the raising and lowering operators $b_n^\dagger(0), b_n(0)$.

2. Alternative expressions for $\|\vec{\gamma}_0'\|$

In this section we derive similar expressions to those of section A 1 for $\|\vec{\gamma}_0'\|$ appearing in theorem 2. One may wonder whether $\{\hat{x}_n, \hat{p}_n\}_{n=1}^\infty$ and $\{\hat{x}_n', \hat{p}_n'\}_{n=1}^\infty$ (defined in Eqs. (16), (24) respectively) are related via a unitary transformation of the form discussed in section A 1 a and thus whether $\|\vec{\gamma}_0'\|$ and $\|\vec{\gamma}_0\|$ are equal. This turns out not to be the case as we will now discover .

a. Relationship between $\vec{\gamma}_0$ and $\vec{\gamma}'_0$

From Eqs. (158) and (161) in[37], one can easily verify using the orthogonality and completeness relations of the underlying orthogonal polynomials that $\vec{R}' = \vec{C}\vec{R}$, $\vec{R}' := (\hat{x}'_1, \hat{x}'_2, \ldots, \hat{p}'_1, \hat{p}'_2, \ldots)^\top$, $\vec{R} := (\hat{x}_1, \hat{x}_2, \ldots, \hat{p}_1, \hat{p}_2, \ldots)^\top$, where

$$\vec{C} = \begin{pmatrix} \vec{A} & \vec{0} \\ \vec{0} & \vec{B} \end{pmatrix}, \tag{A16}$$

with

$$\begin{aligned} [\vec{A}]_{n,m} &= \sqrt{\frac{2}{\omega_{max}}} \int \mu_0(dx) x P'_n(x^2) P_m(x), \\ [\vec{B}]_{n,m} &= \sqrt{2\,\omega_{max}} \int \mu_0(dx) P'_n(x^2) P_m(x). \end{aligned} \tag{A17}$$

This gives us the relation

$$\vec{\gamma}'_0 = \vec{C}\vec{\gamma}_0\vec{C}^\top, \tag{A18}$$

and one can easily verify that $\vec{C}$ satisfies

$$\vec{C}^\top\vec{\Omega}\vec{C} = \vec{\Omega}, \quad \vec{\Omega} := \begin{pmatrix} \vec{0} & \vec{\mathbb{1}} \\ -\vec{\mathbb{1}} & \vec{0} \end{pmatrix}. \tag{A19}$$

However, since $\vec{A}$ and $\vec{B}$ are manifestly not unitary, $\vec{C}$ does not satisfy $\vec{C}\vec{C}^\dagger = \vec{C}^\dagger\vec{C} = \mathbb{1}$ and thus $\vec{\gamma}'_0$, $\vec{\gamma}_0$ are not unitarily equivalent. Therefore, there is no reason to believe that $\|\vec{\gamma}'_0\|$ and $\|\vec{\gamma}_0\|$ are equal in general.

b. Alternative expression for $\vec{\gamma}'_0$

Similarly to section A 1 b, we find that $\vec{\gamma}'_0$ is self-adjoint. Therefore

$$\|\vec{\gamma}'_0\| = \sup_{\|\vec{v}\|=1} \langle \vec{\gamma}'_0\vec{v}, \vec{v}\rangle, \tag{A20}$$

where $\langle \vec{\gamma}'_0\vec{v}, \vec{v}\rangle = \vec{x}'^\top\vec{\gamma}'_{xx}\vec{x} + \vec{p}^\top\vec{\gamma}'_{px}\vec{x} + \vec{x}^\top\vec{\gamma}'_{xp}\vec{p} + \vec{p}^\top\vec{\gamma}'_{pp}\vec{p}$, with $\vec{v} = \vec{x} \oplus \vec{p} \in \mathbb{R}^\infty$. Using (16) and the linearity of the trace, we can write this as

$$\begin{aligned} \langle \vec{\gamma}'_0\vec{v}, \vec{v}\rangle =& \omega_{max} \operatorname{tr}[\hat{x}(f_{1,\vec{x}})\, \hat{x}(f_{1,\vec{x}})\hat{\varrho}_0] + \operatorname{tr}[\hat{p}(f_{2,\vec{p}})\, \hat{x}(f_{1,\vec{x}})\hat{\varrho}_0] \\ &+ \operatorname{tr}[\hat{x}(f_{1,\vec{x}})\, \hat{p}(f_{2,\vec{p}})\hat{\varrho}_0] + \frac{1}{\omega_{max}} \operatorname{tr}[\hat{p}(f_{2,\vec{p}})\, \hat{p}(f_{2,\vec{p}})\hat{\varrho}_0], \end{aligned} \tag{A21}$$

where we have used the notation of Eq. (A1) and defined

$$f_{1,\vec{z}} = f_{1,\vec{z}}(x) = \sum_{k=1}^{\infty} P'_{k-1}(x^2) z_k, \tag{A22}$$

$$f_{2,\vec{z}} = f_{2,\vec{z}}(x) = x f_{1,\vec{z}}(x), \quad \vec{z} = \vec{x}, \vec{p}. \tag{A23}$$

Since $\{P'_n\}_{n=0}^{\infty}$ form a complete orthogonal system, for every function $g \in L^2(\mu_1(dx))$ we can associate uniquely (once a sign convention for the set $\{P'_n\}_{n=0}^{\infty}$ has been chosen) a vector $\vec{g}' \in \mathbb{N}^{\infty}$. This is achieved by writing g in the form

$$g(x) = \sum_{n=1}^{\infty} g'_n P'_{n-1}(x), \tag{A24}$$

from which it follows from the orthogonality relations

$$\int \mu_1(dx) g^2(x) = \|\vec{g}'\|^2 < \infty \quad \text{iff } g \in L^2(\mu_1). \tag{A25}$$

By defining the sets

$$\begin{aligned} S_{\text{even}} &:= \Big\{ f \;\Big|\; \exists\, f' \in L^2(\mu_1)\, s.t.\, f'(x^2) = f(x) \Big\}, \\ S_{\text{odd}} &:= \Big\{ f \;\Big|\; \exists\, f' \in L^2(\mu_1)\, s.t.\, x f'(x^2) = f(x) \Big\}, \end{aligned} \tag{A26}$$

we see that $f_{1,\vec{Z}} \in S_{\text{even}}$ and $f_{2,\vec{Z}} \in S_{\text{odd}}$ iff $\|\vec{z}\| < \infty$. For every $g \in S_{\text{even}}$, and $h \in S_{\text{odd}}$ we associate uniquely (once a sign convention for the set $\{P'_n\}_{n=0}^{\infty}$ has been chosen) a vector $\vec{g}^e \in \mathbb{N}^{\infty}$ and $\vec{h}^o \in \mathbb{N}^{\infty}$ respectively. This is achieved by writing g and h in the form

$$g(x) = \sum_{n=1}^{\infty} g^e_n P'_{n-1}(x^2), \quad h(x) = \sum_{n=1}^{\infty} h^o_n x P'_{n-1}(x^2). \tag{A27}$$

From Eqs. (A24), (A25) and definitions (A26) it follows that the associated vectors $\vec{g}^e$, $\vec{h}^o$ with every $g \in S_{\text{even}}$ and $h \in S_{\text{odd}}$ respectively satisfy $\|\vec{g}^e\| < \infty$ and $\|\vec{h}^o\| < \infty$. Note that for every $g \in S_{\text{even}}$ its associated vector satisfies

$$\begin{aligned} 2 \int \mu_0(dx) x g^2(x) &= \sum_{n,m=1}^{\infty} g^e_n g^e_m 2 \int dx \frac{J(x)}{\pi} x P'_n(x^2) P'_m(x^2) \\ &= \sum_{n,m=1}^{\infty} g^e_n g^e_m \int \mu_1(dy) P'_n(y) P'_m(y) = \sum_{n=0}^{\infty} (g^e_n)^2 = \|\vec{g}^e\|^2, \end{aligned} \tag{A28}$$

where we used the change of variable $y = x^2$. With this observation in mind, we define the set

$$S_{\text{even}}(E) := \Big\{ f \in S_{\text{even}} \Big|\, 2 \int \mu_0(dx) x f^2(x) = E \Big\}. \tag{A29}$$

From Eq. (A28) it follows that $g \in S_{\text{even}}$ is in $S_{\text{even}}(E)$ iff its associated vector $\vec{g}^e$ satisfies $\|\vec{g}^e\|^2 = E$. Similarly to Eq. (A28) we find for every $h \in S_{\text{odd}}$,

$$2\int \mu_0(dx)h^2(x)/x = \|\vec{h}^o\|^2 \tag{A30}$$

and thus we define the set

$$S_{\text{odd}}(E) := \Big\{ f \in S_{\text{odd}} \Big| \, 2\int \mu_0(dx) f^2(x)/x = E \Big\}, \tag{A31}$$

finding that $g \in S_{\text{odd}}$ is in $S_{\text{odd}}(E)$ iff its associated vector $\vec{g}^o$ satisfies $\|\vec{g}^o\|^2 = E$. Thus noting that $\|\vec{v}\|^2 = \|\vec{x}\|^2 + \|\vec{p}\|^2$, from Eqs. (A20), (A21) it follows

$$\begin{aligned} \|\vec{\gamma}_0'\| = \sup_{\substack{f_1 \in S_{\text{even}}(E),\\ f_2 \in S_{\text{odd}}(1-E),\\ E \in [0,1]}} & \Big(\omega_{max} \operatorname{tr}[\hat{x}(f_1)\, \hat{x}(f_1) \hat{\varrho}_0] + \operatorname{tr}[\hat{p}(f_2)\, \hat{x}(f_1) \hat{\varrho}_0] \\ & + \operatorname{tr}[\hat{x}(f_1)\, \hat{p}(f_2) \hat{\varrho}_0] + \frac{1}{\omega_{max}} \operatorname{tr}[\hat{p}(f_2)\, \hat{p}(f_2) \hat{\varrho}_0] \Big). \end{aligned} \tag{A32}$$

Eq. (A32) demonstrates that $\|\vec{\gamma}_0'\|$ can also be calculated by taking the supremum over functions f_1, f_2 in an appropriately defined space.

c. Examples for $\|\vec{\gamma}_0'\|$

This section will follow very closely the example of section A 1 c and will use notation defined there. It is useful to write $\hat{\varrho}_{\text{B}}$ the terms of the local number basis of the raising and lowering operators $b_n^\dagger(1), b_n(1)$ defined in section VI. This basis was first introduced on page 165 of[37], and forms a complete basis for quantum states on $\mathcal{B}$. For every $n \in \mathbb{N}_0$, its associated number basis is generated by the usual relation $b_n(1)|0\rangle_n = 0$, $b_n^\dagger(1)|m\rangle_n' = \sqrt{m+1}|m+1\rangle_n'$. Let us define the state

$$\hat{\varrho}_{\text{B}} = \hat{\rho}_0' \otimes \hat{\rho}_1' \otimes \hat{\rho}_2' \ldots, \tag{A33}$$

where $\hat{\rho}_n' = |n_0\rangle_n' \langle n_0|', \; n \in \mathbb{N}_0$. For $\hat{\varrho}_{\text{B}}$ in Eq. (A33), Eq. (23) takes the form,

$$\vec{\gamma}_0' = \begin{pmatrix} (n_0 + 1/2)\mathbb{1} & (\mathrm{i}/2)\mathbb{1} \\ (-\mathrm{i}/2)\mathbb{1} & (n_0 + 1/2)\mathbb{1} \end{pmatrix}. \tag{A34}$$

As noted in section A 1 c, the two degenerate eigenvalues of Eq. (A34) are n_0 and $n_0 + 1$ and we thus find

$$\|\vec{\gamma}_0'\| = n_0 + 1. \tag{A35}$$

We note that although the r.h.s. of Eqs. (A15) and (A35) are the same, the examples are very different since the states defined in Eqs. (A13) and (A33) are different states. This is because they are defined in different basis. For example, the state in Eq. (A33) for $n_0 = 0$ is *not* the vacuum state of $d\hat{\Gamma}(G)$.